

Time evolution of a quantum many-body system: transition from integrability to ergodicity in thermodynamic limit

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Numerical evidence is given for non-ergodic (non-mixing) behavior, exhibiting ideal transport, of a simple non-integrable many-body quantum system in the thermodynamic limit, namely kicked t - V model of spinless fermions on a ring. However, for sufficiently large kick parameters t and V we recover quantum ergodicity, and normal transport, which can be described by random matrix theory.

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A simple question is addressed here: “Do mixed quantum many-body systems, which are neither integrable nor ergodic, exist in the thermodynamic limit?” While it is clear that integrable systems are rather exceptional it is an important open question whether a finite generic perturbation of an integrable system becomes ergodic or not in the thermodynamic limit (TL), $size \rightarrow \infty$ and *fixed density*. It is known that local statistical properties of quantum systems with few *degrees of freedom* whose classical limit is completely chaotic — *ergodic* are universally described by *random matrix theory*, while in the other extreme case of *integrable* systems Poissonian statistics may typically be applied [1,2]. This statement has recently been verified numerically also for integrable and *strongly* non-integrable many-body systems of interacting fermions [3] which do not have classical limit.

Having lost the reference to classical dynamics we resort to the definition of *quantum ergodicity* (also termed *quantum mixing*) [4] as the decay of time-correlations $\langle A(\tau)B(0) \rangle - \langle A \rangle \langle B \rangle$ of any pair of quantum observables A and B in TL, taking the time-limit $\tau \rightarrow \infty$ in the end. In [4] many-body system of interacting bosons has been studied and it has been shown that quantum ergodicity corresponds to strongly chaotic (classically ergodic) dynamics of associated non-linear mean-field equations. As a consequence of linear response theory, quantum ergodicity also implies normal transport and *finite* transport coefficients (such as dc electrical conductivity). On the other hand, *integrable systems*, which are solvable by Bethe ansatz or quantum inverse scattering, are characterized by (infinitely many) conservation laws and are thus *non-ergodic*. It has been pointed out recently [5] that integrability implies nonvanishing stiffness, i.e. ideal conductance with infinite transport coefficients (or ideal insulating state). As we argue below, any deviation from quantum ergodicity generically implies nonvanishing long-time current auto-correlation and therefore infinite transport coefficient. Since generic non-integrable

systems of finite size (number of degrees of freedom) are non-ergodic (obeying *mixed* statistics smoothly interpolating from Poissonian to random matrix results) it is thus an important question if and when such non-ergodicity can survive TL.

In this Letter we introduce a family of simple many-body systems smoothly interpolating between integrable and ergodic regime, namely *kicked t - V model* (KtV) of spinless fermions with periodically switched nearest neighbor-interaction on a 1-dim lattice of size L and periodic b.c. $L \equiv 0$, with time-dependent hamiltonian

$$H(\tau) = \sum_{j=0}^{L-1} \left[-\frac{1}{2}t(c_j^\dagger c_{j+1} + h.c.) + \delta_p(\tau)Vn_j n_{j+1} \right], \quad (1)$$

and give numerical evidence for the existence of *mixed regime* (reader should not confuse it with *mixing*) in TL by direct simulation of the time evolution. c_j^\dagger, c_j, n_j are fermionic creation, annihilation and number operators, respectively, and $\delta_p(\tau) = \sum_{m=-\infty}^{\infty} \delta(\tau - m)$. Deviations from quantum ergodicity (or mixing) are characterized by several different quantities as described below.

KtV model (1) is a many-body analogue of popular 1-dim non-integrable kicked systems [2] such as e.g. kicked rotor: its evolution (Floquet) operator over one period $U = \hat{T} \exp(-i \int_{0+}^{1+} d\tau H(\tau))$ ($\hbar = 1$), factorizes into the product of kinetic and potential part

$$U = \exp \left(-iV \sum_{j=0}^{L-1} n_j n_{j+1} \right) \exp \left(it \sum_{k=0}^{L-1} \cos(sk + \phi) \tilde{n}_k \right) \quad (2)$$

where $s = 2\pi/L$. Flux parameter ϕ is used in order to introduce a *current operator* $J = (i/t)U^\dagger \partial_\phi U|_{\phi=0} = \sum_{k=0}^{L-1} \sin(sk) \tilde{n}_k$, elsewhere we put $\phi := 0$. Tilde denotes the operators which refer to *momentum* variable k , $\tilde{c}_k = L^{-1/2} \sum_{j=0}^{L-1} \exp(isjk) c_j$, $\tilde{n}_k = \tilde{c}_k^\dagger \tilde{c}_k$. KtV model is integrable if either $t = 0$, or $V = 0 \pmod{2\pi}$, or $tV \rightarrow 0$ and t/V finite (continuous time t - V model, see e.g. [6]), while for $t \sim V \sim 1$ it is expected to be non-integrable, either *quantum ergodic* or *mixed*.

We expect that unitary many-body quantum maps, such as (2), also mimic the dynamics of generic *autonomous* quantum many-body systems on the energy shell in a similar way as 1-dim quantum maps describe (quantum) Poincaré sections of 2-dim quantum (chaotic) systems (see e.g. [8]).

The total number of particles $N = \sum_j n_j$ is conserved, so the map U acts over Hilbert (Fock) space \mathcal{H} of dimension $\mathcal{N} = \binom{L}{N}$. The dynamics of a given initial many body state $|\psi(0)\rangle$, which is an iteration of the map $|\psi(m)\rangle = U|\psi(m-1)\rangle = U^m|\psi(0)\rangle$, can be performed most efficiently by observing that the kinetic part U_T is diagonal in the momentum basis $|\vec{k}\rangle = \tilde{c}_{k_1}^\dagger \cdots \tilde{c}_{k_N}^\dagger |0\rangle$, $k_1 < \dots < k_N$ while the potential part U_V is diagonal in the position basis $|\vec{j}\rangle = c_{j_1}^\dagger \cdots c_{j_N}^\dagger |0\rangle$, $j_1 < \dots < j_N$. The transformation between the two, $F_{\vec{j}\vec{k}} = \langle \vec{j} | \vec{k} \rangle$, is an antisymmetrized N-dim discrete Fourier transformation (DFT) on L-sites which has been efficiently coded in $\sim \mathcal{N} \log_2 \mathcal{N}$ floating point operations (FPO) by factorizing L -site DFT to the product of $\mathcal{O}(L \log_2 L)$ 2-site transformations parametrized with 2×2 sub-matrices $(\alpha, \beta; \gamma, \delta)_{jj'}$, which are successively applied to creation operators, $(c_j^\dagger, c_{j'}^\dagger) \leftarrow (\alpha c_j^\dagger + \beta c_{j'}^\dagger, \gamma c_j^\dagger + \delta c_{j'}^\dagger)$, in all slater determinants $\Pi_n c_{j_n}^\dagger |0\rangle$ which contain a particle at sites j or j' . Our algorithm (fermionic FFT) requires almost no extra storage apart from a vector of \mathcal{N} c-numbers and works for lattices of sizes $L = 2^p, 10, 12, 15, 20, 24, 30, 40$. Therefore, the map (2) is iterated on a vector $\psi_{\vec{k}}(m) = \langle \vec{k} | \psi(m) \rangle$, using the matrix composition $U = F^* U_V F U_T$ in roughly $2\mathcal{N} \log_2 \mathcal{N}$ FPO per time step which is by far superior to complete diagonalization techniques ($\mathcal{O}(\mathcal{N}^3)$ FPO), even for *long* time scales $m = \mathcal{O}(\mathcal{N})$ when quantum dynamics becomes quasiperiodic due to discreteness of the spectrum of U .

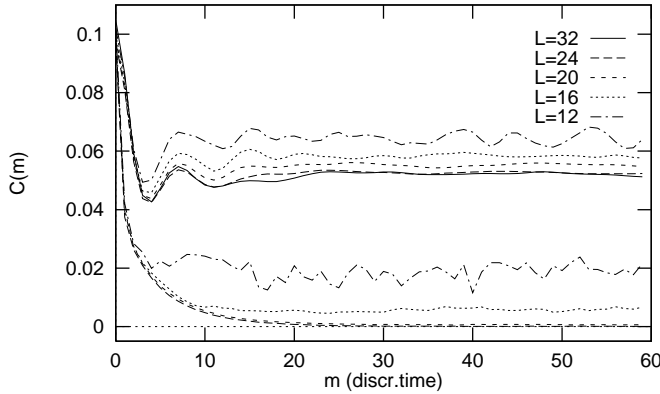


FIG. 1. Current autocorrelation function $C_J(m)$ against discrete time m for quantum ergodic ($t = V = 4$, lower set of curves for various sizes L) and mixed regime ($t = V = 1$, upper set of curves) with density $\rho = \frac{1}{4}$. Averaging over entire Fock space is performed, $\mathcal{N}' = \mathcal{N}$, for $L \leq 20$, whereas random samples of $\mathcal{N}' = 12000$, and $\mathcal{N}' = 160$ initial states have been used for $L = 24$, and $L = 32$, respectively.

First we consider decay of current autocorrelation function $C_J(m) = (1/L) \langle J(m)J(0) \rangle$ where $J(m) = U^{\dagger m} J U^m$, and $\langle \cdot \rangle = (1/\mathcal{N}) \text{Tr}(\cdot)$ is a ‘microcanonical average’. Note that J is diagonal in the momentum basis $J|\vec{k}\rangle = J_{\vec{k}}|\vec{k}\rangle$, and $\langle J \rangle = 0$. So $C_J(m)$ can be evaluated

by means of time-evolution of momentum initial states $|\psi(0)\rangle = |\vec{k}'\rangle$

$$C_J(m) = \frac{1}{L\mathcal{N}'} \sum_{\vec{k}'} J_{\vec{k}'} \sum_{\vec{k}} J_{\vec{k}} p_{\vec{k}\vec{k}'}(m) \quad (3)$$

where $p_{\vec{k}\vec{k}'}(m) = |\langle \vec{k} | \psi(m) \rangle|^2 = |\langle \vec{k} | U^m | \vec{k}' \rangle|^2$. For large sizes L , a smaller but uniformly random sample of \mathcal{N}' initial states $|\vec{k}'\rangle$, $1 \ll \mathcal{N}' \ll \mathcal{N}$, is used in order to save computer time. Direct computation of $C_J(m)$ for $m \leq M$ can be performed in $\sim (2MN\mathcal{N}'/L) \log_2 \mathcal{N}$ FPO, since due to translational symmetry one can simultaneously simulate the dynamics of L different states with different values of the conserved total momentum $K = \sum_n k'_n \pmod{L}$. Using the eigenphases η_n and eigenstates $|n\rangle$ of evolution operator U , $U|n\rangle = e^{-i\eta_n}|n\rangle$, $n = 1 \dots \mathcal{N}$, one can write *dissipative* dc conductivity of such a kicked system $\sigma := \sum_{n=1}^{\mathcal{N}} (\partial_\phi \eta_n)^2 \approx C_J(0) + 2 \sum_{m=1}^{\mathcal{N}/2} C_J(m)$. Note that $\partial_\phi \eta_n = \langle n | J | n \rangle$.

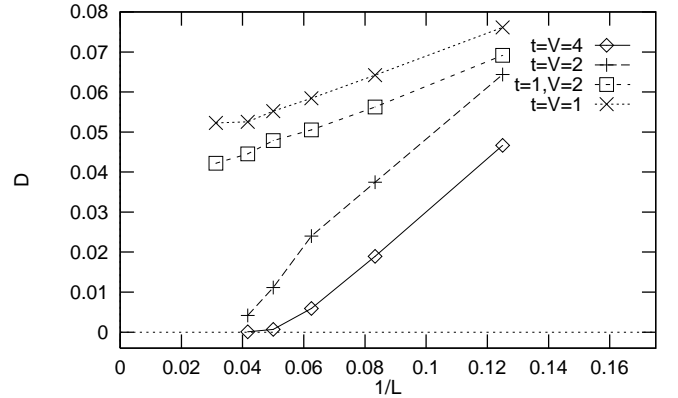


FIG. 2. Stiffness D_J vs. $1/L$ at constant density $\rho = \frac{1}{4}$ and for different values of control parameters in ergodic, $t = V = 4$ and $t = V = 2$, and mixed, $t = 1, V = 2$ and $t = V = 1$, regime. Other parameters are the same as in fig.1.

In fig.1 we present numerical computation of correlation function $C_J(m)$ for parameters $t = V = 1$ and $t = V = 4$, for various sizes L , but at fixed density $\rho = N/L = \frac{1}{4}$. Quite generally, $C_J(m)$ exhibits fast relaxation on a time scale M^* which is typically small, $M^* \sim 10$, and roughly independent of L , and afterwards it fluctuates around averaged limiting value, the *stiffness*

$$D_J = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{m=1}^M C_J(m) \quad (4)$$

where the strength of fluctuations decreases with increasing size L . Note again that TL $L \rightarrow \infty$ should be taken prior to the time-limit, $\lim_{M \rightarrow \infty} (1/M) \sum_{m=1}^M (\cdot)$, which is for systems of finite size L here and below estimated numerically as $(1/M') \sum_{m=M'+1}^{2M'} (\cdot)$ with sufficiently large but fixed averaging time $M' > M^*$; we

take $M' = 30$. If the system is quantum ergodic (case $t = V = 4$ of fig.1), D_J goes to zero and σ remains finite as $L \rightarrow \infty$ ($\mathcal{N} \rightarrow \infty$) and $\rho = N/L$ fixed, whereas in the other case ($t = V = 1$ of fig.1) D_J remains well above zero as we approach TL whereas conductivity σ diverges [7]. In fig.2 we have analyzed the scaling of D_J with $1/L$. For large values of parameters, say $t = V = 4$, D_J is practically zero already for $L \approx 20$, while for smaller (but not small) control parameters (t, V), $D_J \approx D_J^\infty + \beta/L$ where $D_J^\infty > 0$. In *close-to-critical* case $t = V = 2$, we find larger correlation time $M^* \sim 10^2$, and hence use longer averaging time $M' = 200$. In fig.3 we illustrate an *ideal transport* for $t \sim V \sim 1$ by plotting a *persistent current* $J_{\vec{k}'}^p = \lim_{M \rightarrow \infty} (1/M) \sum_{m=1}^M \langle \vec{k}' | J(m) | \vec{k}' \rangle$ vs. the initial current $J_{\vec{k}'}$. The normal transport in the ergodic regime $t = V = 4$ is characterized by $J_{\vec{k}'}^p = 0$, while for $t \sim V \sim 1$ we find ideal transport with the persistent current being proportional to the initial current, $J_{\vec{k}'}^p = \alpha J_{\vec{k}'}$. Proportionality constant α can be computed from (4) $D_J = (1/L) \langle J_{\vec{k}'} J_{\vec{k}'}^p \rangle = (\alpha/L) \langle J^2 \rangle$, so $\alpha = 2D_J / [\rho(1-\rho)]$, where $\langle J^2 \rangle$ is given below (5).

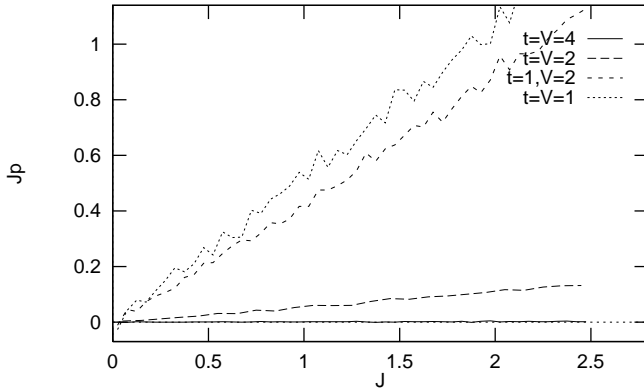


FIG. 3. Persistent current $J_{\vec{k}}^p$ against initial current $J_{\vec{k}}$ (averaged over bins of size $\Delta J = 0.005$) in the ergodic $t = V = 4$, (nearly) ergodic $t = V = 2$, and mixed regime, $t = V = 1$ and $t = 1, V = 2$. In all cases, $L = 24$ and $\rho = \frac{1}{4}$.

Due to translational symmetry the total momentum $K = \sum_k k \tilde{n}_k \pmod{L}$ is the only conserved quantity (apart from N and parity), so the evolution of initial momentum state $|\vec{k}'\rangle$ takes place in $\mathcal{N}_K \approx \mathcal{N}/L$ dim. subspace \mathcal{H}_K , spanned by $|\vec{k}\rangle$ with $K = |\vec{k}| := \sum_n k_n$. Starting with a momentum state $|\vec{k}'\rangle$, the number of ‘excited’ states $|\vec{k}\rangle$ after time m is characterized by information entropy [9] (see also [8]) as $\exp(-\sum_{\vec{k}} p_{\vec{k}\vec{k}'}(m) \log p_{\vec{k}\vec{k}'}(m))$. Averaging the entropy over uniformly random sample of \mathcal{N}' initial states $|\vec{k}'\rangle$ we define *relative localization dimension* in Fock space as a measure of quantum ergodicity.

$$R(m) = \frac{L}{\mathcal{N}} \exp \left(-\frac{1}{\mathcal{N}'} \sum_{\vec{k}'} \sum_{\vec{k}} p_{\vec{k}\vec{k}'}(m) \log p_{\vec{k}\vec{k}'}(m) \right).$$

Again similar behavior is found numerically for $R(m)$ as for $C_J(m)$ (the two quantities can be computed simultaneously at no extra cost), namely it typically saturates within the same (short) correlation time M^* to a roughly constant value $\bar{R} = \lim_{M \rightarrow \infty} (1/M) \sum_{m=1}^M R(m)$

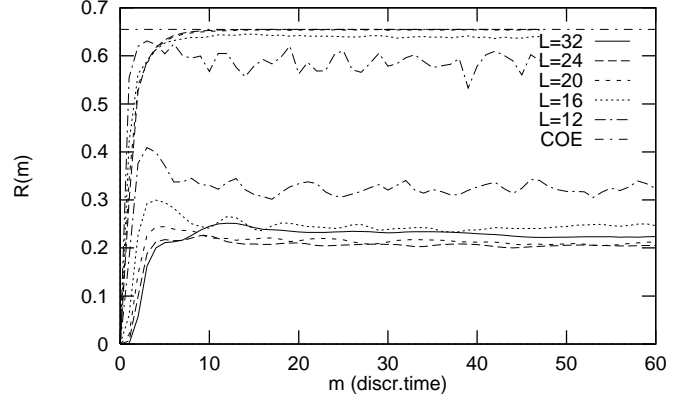


FIG. 4. Relative localization dimension in Fock space, $R(m)$ for data of fig.1.

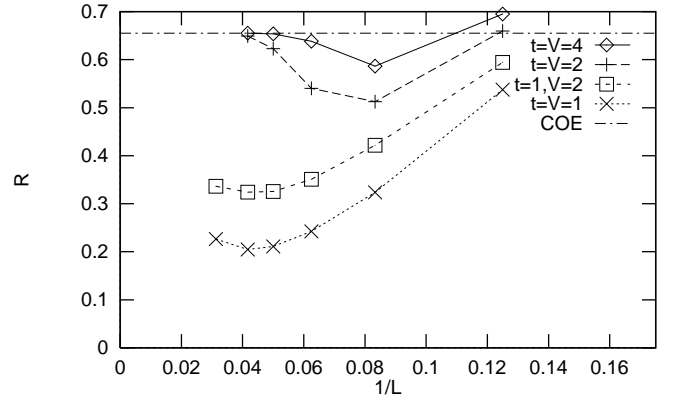


FIG. 5. Limiting rel.loc.dim. \bar{R} vs. $1/L$ for data of fig.2.

If there are no additional, even approximate conservation laws the blocks $U^m|_{\mathcal{H}_K}$ may be modeled by circular orthogonal ensemble (COE) of random matrices for sufficiently large m giving the maximal asymptotic (as $\mathcal{N} \rightarrow \infty$) value of relative localization dimension, $\bar{R}_{COE} \approx 0.655$. This case corresponds to quantum ergodicity since $p_{\vec{k}\vec{k}'}(m)$, for $m > M^*$, become pseudo random and independent of \vec{k} and \vec{k}' , hence the correlation function (3) factorizes and yields $C(m) = \langle J \rangle^2 = 0$. Indeed, as we show in fig.4, such behavior is obtained only for sufficiently large parameters, say $t = V = 4$, while for smaller values of parameters t, V , $R(m)$ saturates to a smaller value indicating that there may exist approximate conservation laws causing nontrivial localization inside the Fock space. Scaling with $1/L$ suggests that even TL of \bar{R} is smaller than \bar{R}_{COE} for $t \sim V \sim 1$ (fig.5).

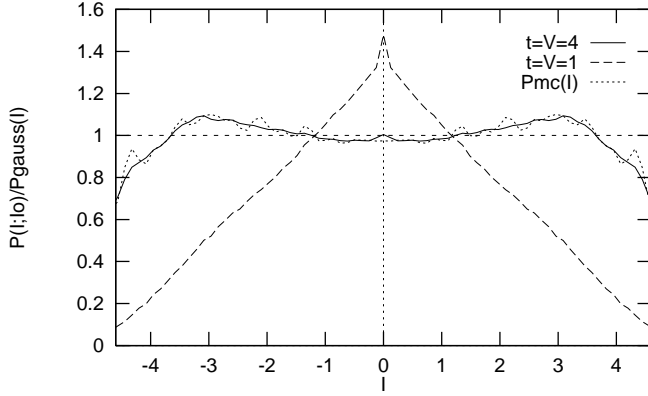


FIG. 6. Steady-state current distribution divided by a gaussian $P(I, I_0)/P_{gauss}(I)$ averaged over 279 initial orbits with $|I_0| < 0.08$ in the ergodic, $t = V = 4$, and mixed, $t = V = 1$, regime, and the finite-size microcanonical current distribution $P_{mc}(I)$. $L = 24$, $\rho = \frac{1}{4}$.

Finally, we discuss current fluctuations, or more generally, current distribution $P_\psi(I) = \langle \psi | \delta(I - J) | \psi \rangle$ giving a probability density of having a current I in a state $|\psi\rangle$. We let the state ψ with a ‘good’ known initial current I_0 to evolve for a long time from which we compute a steady-state current distribution (SSCD)

$$P(I; I_0) = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{m=1}^M \langle \delta(I_0 - J(0)) \delta(I - J(m)) \rangle.$$

Of course, delta functions should have a finite small width providing averaging over several states $|\vec{k}\rangle$ with $J_{\vec{k}} \approx I_0$. In the quantum ergodic regime all states eventually become populated, so SSCD $P(I; I_0)$ should be independent of initial current I_0 and equal to the *microcanonical current distribution* $P_{mc}(I) = \langle \delta(I - J) \rangle$. It has been shown by elementary calculation that in TL the latter becomes a gaussian, $P_{mc}(I) \rightarrow P_{gauss}(I) = (1/\sqrt{2\pi\langle J^2 \rangle}) \exp(-\frac{1}{2}I^2/\langle J^2 \rangle)$, while at any finite size L the first few moments are:

$$\begin{aligned} \langle J^2 \rangle &= \frac{N(L-N)}{2(L-1)} \approx \frac{1}{2}\rho(1-\rho)L, \\ \frac{\langle J^4 \rangle}{\langle J^2 \rangle^2} &= \frac{3(L-1)(2N(L-N)-L)}{2N(L-2)(L-N)} \\ &= 3 + \frac{3(2\rho(1-\rho)-1)}{2\rho(1-\rho)} \frac{1}{L} + \mathcal{O}(L^{-2}). \end{aligned} \quad (5)$$

Numerical results for $L = 24$ (see fig.6) indicate that in the ergodic regime, $t = V = 4$, SSCD is already in good agreement with microcanonical distribution $P_{mc}(I)$, while in non-ergodic (mixed) regime, $t = V = 1$, SSCD is *localized* on a smaller range indicating that the current fluctuation is smaller than $\langle J^2 \rangle$. Note that the mean $\bar{I} = \int dI I P(I; I_0)$ is just a persistent current, so $\bar{I} = \alpha I_0$ (see fig.3).

In this Letter we have presented numerical evidence, based on efficiently coded time evolution of a kicked fermionic system, in support of hypothesis that mixed (neither integrable nor ergodic) behavior of a quantum many-body system may survive TL provided that control parameters are not too far away from integrable points. It has been shown that in this regime ideal transport is possible. However, if the control parameters are sufficiently large we recover quantum ergodicity compatible with random matrix theory and normal transport properties. It is interesting to note that at the transition point between the two regimes, where *order parameter* – *stiffness* $D_J|_{L=\infty}$ (inferred from $1/L$ scaling) touches zero, the correlation time scale M^* drastically increases what is reminiscent of a kind of *dynamical* phase transition. Although only data for quarter-filled lattice ($\rho = \frac{1}{4}$) are presented here, we should stress that essentially the same conclusions follow from our data for other densities, $\rho = \frac{1}{3}, \frac{3}{8}, \frac{2}{5}, \frac{1}{2}$, with a general rule, that the border of quantum ergodic regime moves to slightly smaller values of control parameters t, V as the density ρ approaches $\frac{1}{2}$. It should be noted that statistics of eigenphases of evolution operator U has been computed as well and it has been found that in the ergodic regime level statistics is indeed that of COE while in the mixed regime it smoothly interpolates between Poisson and COE.

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